

# **Risk-Informed Mechanistic Source Term Calculation**

---

*Final CRADA Report*

**Nuclear Science and Engineering**

### **About Argonne National Laboratory**

Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC under contract DE-AC02-06CH11357. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne and its pioneering science and technology programs, see [www.anl.gov](http://www.anl.gov).

### **DOCUMENT AVAILABILITY**

**Online Access:** U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free at OSTI.GOV (<http://www.osti.gov/>), a service of the U.S. Dept. of Energy's Office of Scientific and Technical Information

### **Reports not in digital format may be purchased by the public from the National Technical Information Service (NTIS):**

U.S. Department of Commerce  
National Technical Information Service  
5301 Shawnee Rd  
Alexandria, VA 22312  
**[www.ntis.gov](http://www.ntis.gov)**  
Phone: (800) 553-NTIS (6847) or (703) 605-6000  
Fax: (703) 605-6900  
Email: **[orders@ntis.gov](mailto:orders@ntis.gov)**

### **Reports not in digital format are available to DOE and DOE contractors from the Office of Scientific and Technical Information (OSTI):**

U.S. Department of Energy  
Office of Scientific and Technical Information  
P.O. Box 62  
Oak Ridge, TN 37831-0062  
**[www.osti.gov](http://www.osti.gov)**  
Phone: (865) 576-8401  
Fax: (865) 576-5728  
Email: **[reports@osti.gov](mailto:reports@osti.gov)**

### **Disclaimer**

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor UChicago Argonne, LLC, nor any of their employees or officers, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of document authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, Argonne National Laboratory, or UChicago Argonne, LLC.

# Risk-Informed Mechanistic Source Term Calculation

---

*Final CRADA Report*

Prepared by  
David Grabaskas, Matthew Bucknor, Yiqi Yu, Elia Merzari, Michael Billone  
Nuclear Science and Engineering Division, Argonne National Laboratory

James Jerden  
Chemical and Fuel Cycle Technologies Division, Argonne National Laboratory

Participants: John Hanson, Alexandra Popova Renner, Joshua Richard  
Oklo Inc.

September 2019

*This page intentionally left blank*

## Non Proprietary Final CRADA Report

For the Office of Scientific and Technical Information (OSTI)

**CRADA Number:** 2017-17153

**CRADA Title:** Risk-Informed Mechanistic Source Term Calculation

**CRADA Start Date** 6/27/2018 – **End Date** 8/31/2019

### DOE Program or Other Government Support

**Program office:** DOE: Nuclear Energy

**Program manager name:** John Jackson

**Program manager phone or email:** john.jackson@inl.gov

### Participant(s)

**Participant 1 name:** Oklo Inc.

**Complete address:** 203 E. Caribbean Dr., Sunnyvale CA

### Argonne National Laboratory

Argonne PI(s): David Grabaskas

### Funding Table

To add rows, right-click in bottom row and select "Insert" "rows above".

	Planned Funding	Actual Funding	In-Kind
Government	216,000\$	216,000\$	
Oklo Inc.	0\$	0\$	57,000\$
<b>Total</b>	<b>216,000\$</b>	<b>216,000\$</b>	<b>57,000\$</b>

### Nature of Work

**Describe the research (summary of Scope of Work and principal objectives of the CRADA):**

See following report.

### DOE mission area(s):

Energy and Environmental Science and Technology

### Conclusions drawn from this CRADA; include any major accomplishments:

Three major tasks were completed as part of the CRADA. First, a coupling strategy was developed and demonstrated for an integrated high fidelity analysis of radial core expansion utilizing the Nek5000, Diablo, and OpenMC codes. Second, a mechanistic source term analysis, which realistically evaluates the potential radionuclide release to the environment during transient event sequences, was performed for a reactor design under consideration by Oklo. Lastly, past fuel performance data from the Argonne EBR-II reactor was analyzed to support a regulatory fuel qualification effort.

### Technology Transfer-Intellectual Property

**Argonne National Laboratory background IP:**

Fuel performance data from the Argonne EBR-II reactor.

### Participant(s) background IP:

Oklo reactor design information.

**Identify any new Subject Inventions as a result of this CRADA:**

N/A

**Summary of technology transfer benefits to industry and, if applicable, path forward/anticipated next steps towards commercialization:**

The CRADA assisted in three areas related to regulatory reactor licensing. This includes an approach to evaluate the reactor core response to changes in temperature (high-fidelity radial core expansion analysis), a mechanistic evaluation of the potential consequences associated with transient event sequences, and supporting information for the qualification of reactor fuel.

**Other information/results (papers, inventions, software, etc.):**

N/A

## Table of Contents

<b>1 INTRODUCTION .....</b>	<b>2</b>
<b>2 TASK 1: NEK5000, DIABLO, AND OPENMC COUPLING.....</b>	<b>3</b>
<b>3 TASK 2: MECHANISTIC SOURCE TERM ANALYSIS .....</b>	<b>5</b>
<b>4 TASK 3: METAL FUEL QUALIFICATION.....</b>	<b>7</b>
<b>BIBLIOGRAPHY .....</b>	<b>8</b>

## 1 Introduction

As part of an FY18 U.S. Department of Energy (DOE) Gateway for Accelerated Innovation in Nuclear (GAIN) award, a CRADA agreement was established between Argonne National Laboratory (Argonne) and Oklo. The CRADA focused on the following three tasks to assist Oklo with the regulatory licensing of their innovative nuclear reactor design:

- **Task 1 – Coupling and Demonstration Analysis using The Nek5000, Diablo, and OpenMC Codes:** Establishing a coupling between the neutronic, structural, and thermo-hydraulic analysis codes and utilizing the code package for a high-fidelity demonstration analysis of radial core expansion due to temperature changes and its impact on core reactivity.
- **Task 2 – Mechanistic Source Term Analysis:** Performing a realistic evaluation of the potential release of radionuclides to the environment during postulated transient event sequences.
- **Task 3 – Data in Support of Metal Fuel Qualification:** An assessment of past post-irradiation examination data of metal fuel utilized in the Argonne EBR-II reactor to assist in the potential qualification of the fuel typer for regulatory licensing.

The details regarding each analysis and the associated conclusions were provided to Oklo in three separate project reports. Due to the utilization of proprietary and export controlled information, the current summary report was created, which provides an uncontrolled overview of each of the three tasks.

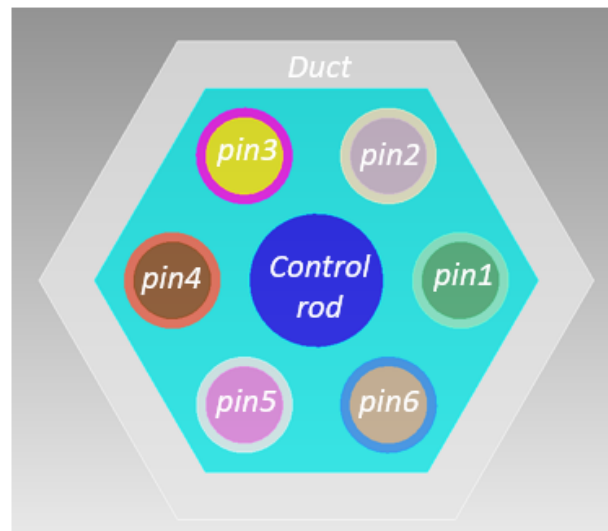


## 2 Task 1: Nek5000, Diablo, and OpenMC Coupling

The first task of the Argonne/Oklo CRADA centered on coupling the OpenMC, Nek5000, and Diablo codes for a demonstration multi-physics simulation of radial core expansion. In general, radial core expansion is caused by the motion of fuel assemblies in response to thermal expansion during temperature changes in the core, which then impacts core reactivity. Therefore, the core restraint system must be carefully designed to ensure that the radial core expansion induces a negative reactivity response and aids in the return of the reactor to a safe operating condition. The desired OpenMC/Nek5000/Diablo toolkit is a multi-physics software package that couples neutronics, computational fluid dynamics, and structural mechanics, allowing for direct modeling of radial and axial core expansion that could previously only be estimated indirectly.

The code integration was based on the Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) toolkit which was developed by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Campaign, with the inclusion of OpenMC, which is a Monte Carlo (MC) neutronics solver. A new coupling strategy was developed for the integration between SHARP and OpenMC, as SHARP is a mesh-based toolkit while OpenMC uses Constructive Solid Geometry (CSG) method.

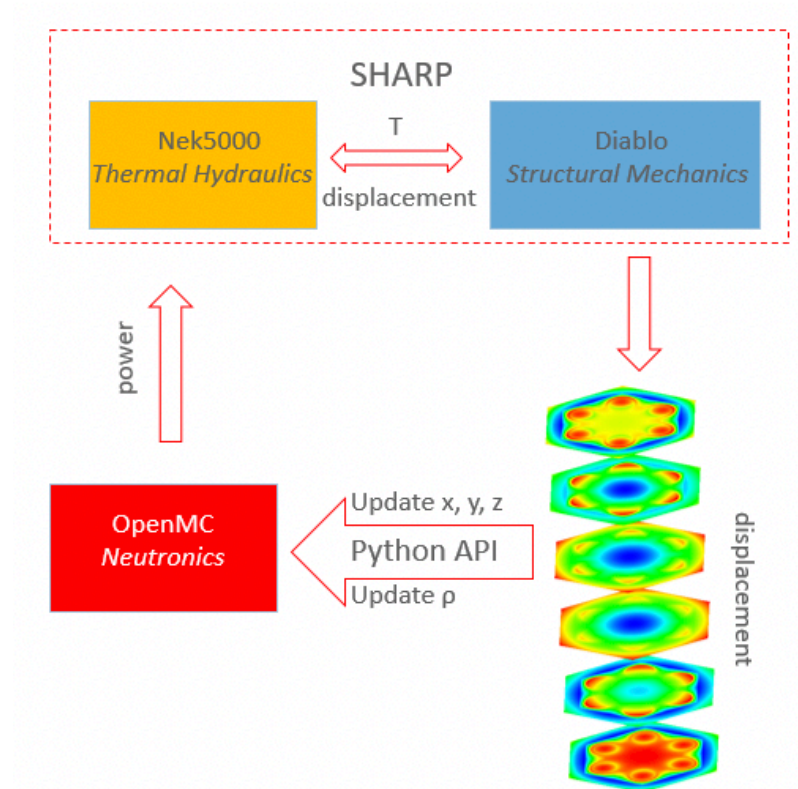
As a demonstration of the coupled toolkit, a radial expansion analysis was performed using an example, simplified core geometry called SAHEX, which consists of a single hexagonal assembly containing six fuel pins with cladding and one central “control” rod. The configuration of the model is shown in Figure 2-1.



**Figure 2-1: Configuration of SAHEX**

The code coupling approach included multiple steps, as outlined in Figure 2-2. As part of the demonstration analysis, sensitivity analyses were performed at each step to ensure accuracy and convergence. An example of a sensitivity study, examining mesh density, found that the results were most sensitive to mesh density in the z-direction, which had to be refined to ensure accurate

rod deformation results. Additional sensitivity studies assessed mesh resolution, isotope composition, and batch and particle number.



**Figure 2-2: Schematic of Coupling Approach between SHARP and OpenMC**

The proposed workflow was demonstrated to be feasible in the performance of multi-physics simulations. The SAHEX problem was assessed with both the SHARP (PROTEUS, Nek5000, Diablo) toolkit and the new package (OpenMC, Nek5000, Diablo). Good agreement was found between the two toolkits for the prediction of the reactivity feedback due to radial expansion. Due to the basic methodology difference between SHARP and OpenMC (i.e., mesh-based vs. CSG), there is a potential for the introduction of error during data transfer. Analyst effort is necessary to perform the required simplifications to reduce error. Although it is difficult to develop a generic approach that is applicable to all potential problems, the methodology utilized for the demonstration analysis serves as a beneficial reference point and experience for future studies.

### 3 Task 2: Mechanistic Source Term Analysis

Recently, Argonne performed several studies regarding the development of mechanistic source term (MST) analyses for metal fuel sodium fast reactors (SFRs). An MST is a realistic assessment of the release and transport of radionuclides from the core fuel through the reactor system and potentially to the environment during transient event sequences. These studies examined radionuclide behavior within the fuel [1], radionuclide transport/retention phenomena [2], and a trial MST analysis was performed utilizing currently available tools and models [3]. The findings of these studies also resulted in the development of a new Argonne MST analysis code [4], described in the following subsection.

Although the Oklo reactor design is not an SFR, there are similarities in the MST analysis due to the potential use of metal fuel, which is a central factor in the determination of radionuclide release during transient event sequences. An MST analysis was performed for a proposed version of the Oklo reactor design utilizing the Argonne Simplified Radionuclide Transport (SRT) code [5]. An overview of the MST analysis and several sensitivity assessments is provided here, as details of the reactor design, analysis assumptions, and results are not included due to proprietary restrictions.

The Argonne SRT code models the release, transport, and retention of radionuclides in SFRs and microreactor systems. As shown in Figure 3-1, SRT does not model the transient behavior of the reactor but utilizes the results of system analysis codes or postulated reactor conditions from the analyst. Using this information, SRT assesses multiple radionuclide behavior phenomena, including the migration of radionuclides within the fuel elements during irradiation, the release of radionuclides from the fuel during cladding failure, radionuclide transport within the reactor vessel and containment, and potential release to the environment and offsite dose.

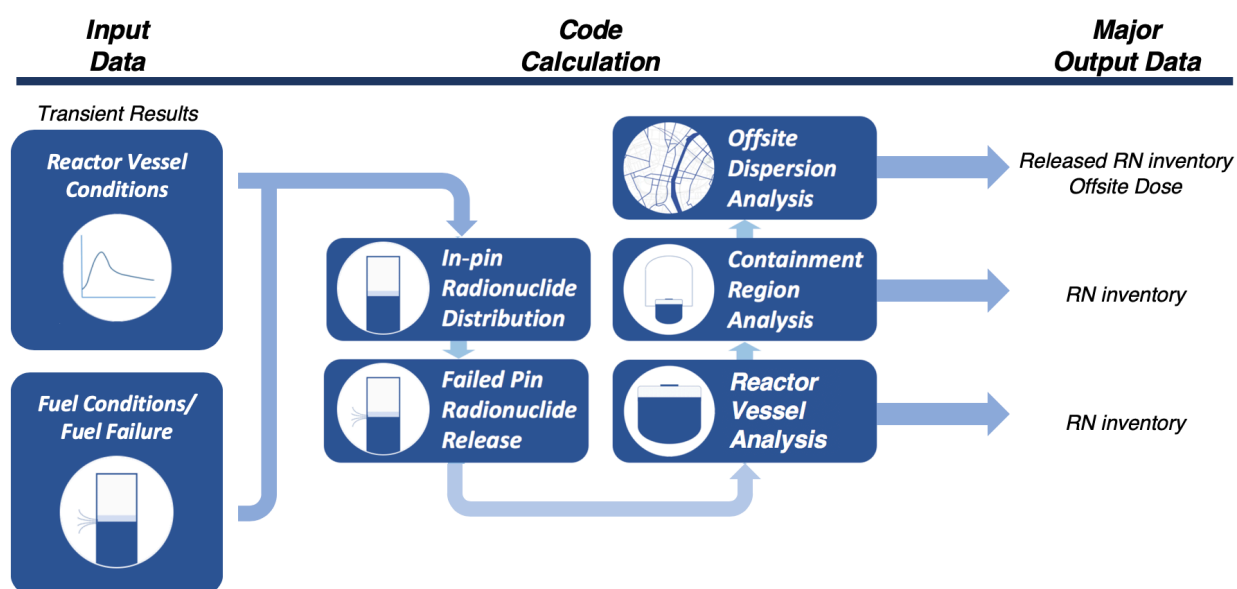


Figure 3-1: SRT Microreactor Source Term Analysis Overview [5]

Multiple SRT analyses were performed to examine potential transient event sequences and assess the importance of particular phenomena or parameters. SRT is purposefully designed to conduct sensitivity and uncertainty analyses, which aided in the identification of high impact variables. Once identified, additional analyses were performed to examine the data available to support the use of the modeling choices and input parameters. Sensitivity analyses also examined offsite dose modeling tools, including a comparison of a simplified  $\chi/Q$  dispersion analysis and a detailed analysis performed with WinMACCS [6]. HSC Chemistry [7] calculations were utilized to support assumptions regarding the chemical and physical state of radionuclides during different phases of the transport process.

The use of the SRT code, in conjunction with supporting analyses, was able to examine the transport and retention of radionuclides for the possible Oklo reactor design during postulated transient event sequences. The results of the analyses not only give insight into the potential offsite dose values and their acceptability for regulatory licensing but also the identification of important phenomena and parameters. The latter of which is important to ensure that there is adequate confidence in the modeling choices and selected variable values to justify their use for licensing calculations.

## 4 Task 3: Metal Fuel Qualification

A major regulatory requirement for reactor licensing is the qualification of the selected fuel type. Fuel qualification can be a challenging task for new reactor developers, as a significant data set is required to provide adequate confidence in fuel performance. The data can be difficult to acquire, as substantial fuel irradiation experience is often necessary. Task 3 of the Argonne/Oklo CRADA focused on supporting information for the qualification of a possible fuel choice for the Oklo reactor design.

Argonne has substantial experience in the development and utilization of metal fuel forms in nuclear reactors. One of the most common metal fuel compositions is U-10Zr, which is a metallic uranium fuel with the inclusion of zirconium. The addition of zirconium increases the solidus temperature of the fuel, providing additional margin during potential transient event sequences. The U.S. has significant U-10Zr fuel irradiation experience (>14,000 fuel pins) in the EBR-II and FFTF reactors.

As part of this task, the available data from an EBR-II U-10Zr fuel experiment were analyzed to assess fuel performance parameters, which could help support a regulatory fuel qualification effort. The metrics assessed included:

- Fuel axial strain: The increase in fuel length during irradiation
- Fuel diametral stain: The increase in fuel diameter during irradiation
- Fission gas release: The increase in fission gas release during irradiation

The chosen experiment also allows an assessment of fuel volume increase (fuel swelling) to be conducted, which is valuable data for the calculation of internal fuel pin pressures and cladding strain/stress. Neutron radiography and additional destructive fuel pin examinations serve as the basis for this data. In total, the fuel performance data from 22 fuel elements was assessed to provide insight into the behavior of a potential fuel choice for the Oklo reactor design.

## Bibliography

- [1] D. Grabaskas, M. Bucknor, and J. Jerden, "Regulatory Technology Development Plan - Sodium Fast Reactor: Mechanistic Source Term - Metal Fuel Radionuclide Release," Argonne National Laboratory,ANL-ART-38, 2016.
- [2] D. Grabaskas, A. J. Brunett, M. Bucknor, J. Sienicki, and T. Sofu, "Regulatory Technology Development Plan - Sodium Fast Reactor: Mechanistic Source Term Development," Argonne National LaboratoryANL-ART-3, 2015.
- [3] D. Grabaskas *et al.*, "Regulatory Technology Development Plan - Sodium Fast Reactor: Mechanistic Source Term Development - Trial Calculation," Argonne National Laboratory,ANL-ART-49, 2016.
- [4] D. Grabaskas, J. Jerden, and M. Bucknor, "A New Computational Tool for Rapid Uncertainty and Sensitivity Analyses of Sodium Reactor Source Term," presented at the 2019 ANS Annual Meeting, 2019.
- [5] D. Grabaskas, M. Bucknor, and J. Jerden, "Simplified Radionuclide Transport (SRT) Code: Users Manual," ANL-SRT-4, 2019.
- [6] Sandia National Laboratories, "WinMACCS, a MACCS2 Interface for Calculating Health and Economic Consequences from Accidental Release of Radioactive Materials into the Atmosphere - User's Guide and Reference Manual WinMACCS Version 3," 2007.
- [7] Outotec, "HSC Chemistry 8 User's Guide," 2014.



**Nuclear Science and Engineering**  
Argonne National Laboratory  
9700 South Cass Avenue, Bldg. 208  
Argonne, IL 60439

[www.anl.gov](http://www.anl.gov)



Argonne National Laboratory is a U.S. Department of Energy  
laboratory managed by UChicago Argonne, LLC